



## Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:15 AM JST

PDB ID : 9VB0 / pdb\_00009vb0  
EMDB ID : EMD-64911  
Title : Cryo-EM structure of human Neurotensin Receptor 1 (hNTSR1)-Gi1 complex  
in nucleotide-free NC state 2  
Authors : Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.;  
Kato, H.E.  
Deposited on : 2025-06-04  
Resolution : 3.19 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

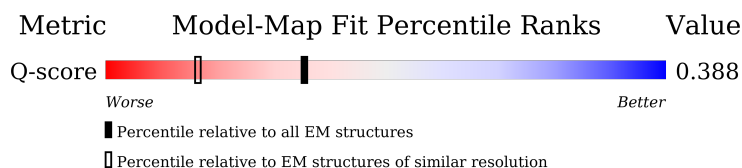
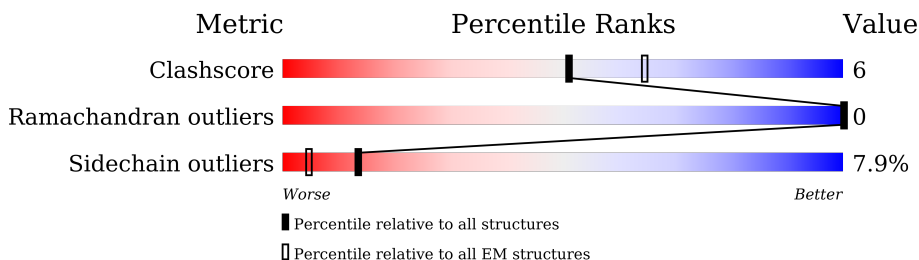
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 ( 2.69 - 3.69 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	354	
2	B	358	
3	C	71	
4	D	259	

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Mol	Chain	Length	Quality of chain
5	R	436	<div><div></div><div>48%</div><div>35%</div><div>19%</div><div>6%</div><div>•</div><div>37%</div></div>
6	L	6	<div><div></div><div>83%</div><div>67%</div><div>33%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8758 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1758	1120	293	333	12		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2585	1596	461	507	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	54	Total	C	N	O	S	0	0
			410	259	71	77	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1762	1121	294	337	10		

- Molecule 5 is a protein called Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	276	Total	C	N	O	S	0	0
			2190	1447	364	365	14		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	MET	-	initiating methionine	UNP P30989
R	-10	GLY	-	expression tag	UNP P30989
R	-9	GLN	-	expression tag	UNP P30989
R	-8	PRO	-	expression tag	UNP P30989
R	-7	GLY	-	expression tag	UNP P30989
R	-6	ASN	-	expression tag	UNP P30989
R	-5	GLY	-	expression tag	UNP P30989
R	-4	SER	-	expression tag	UNP P30989
R	-3	ALA	-	expression tag	UNP P30989
R	-2	PHE	-	expression tag	UNP P30989
R	-1	LEU	-	expression tag	UNP P30989
R	0	LEU	-	expression tag	UNP P30989
R	1	ALA	-	expression tag	UNP P30989
R	2	PRO	-	expression tag	UNP P30989
R	3	ASN	-	expression tag	UNP P30989
R	4	ARG	-	expression tag	UNP P30989
R	5	SER	-	expression tag	UNP P30989
R	6	HIS	-	expression tag	UNP P30989
R	7	ALA	-	expression tag	UNP P30989
R	8	PRO	-	expression tag	UNP P30989
R	9	ASP	-	expression tag	UNP P30989
R	10	HIS	-	expression tag	UNP P30989

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Chain	Residue	Modelled	Actual	Comment	Reference
R	11	ASP	-	expression tag	UNP P30989
R	12	VAL	-	expression tag	UNP P30989
R	13	GLU	-	expression tag	UNP P30989
R	14	ASN	-	expression tag	UNP P30989
R	15	LEU	-	expression tag	UNP P30989
R	16	TYR	-	expression tag	UNP P30989
R	17	PHE	-	expression tag	UNP P30989
R	18	GLN	-	expression tag	UNP P30989
R	19	GLY	-	expression tag	UNP P30989
R	85	LEU	ALA	engineered mutation	UNP P30989
R	419	LEU	-	expression tag	UNP P30989
R	420	GLU	-	expression tag	UNP P30989
R	421	VAL	-	expression tag	UNP P30989
R	422	LEU	-	expression tag	UNP P30989
R	423	PHE	-	expression tag	UNP P30989
R	424	GLN	-	expression tag	UNP P30989

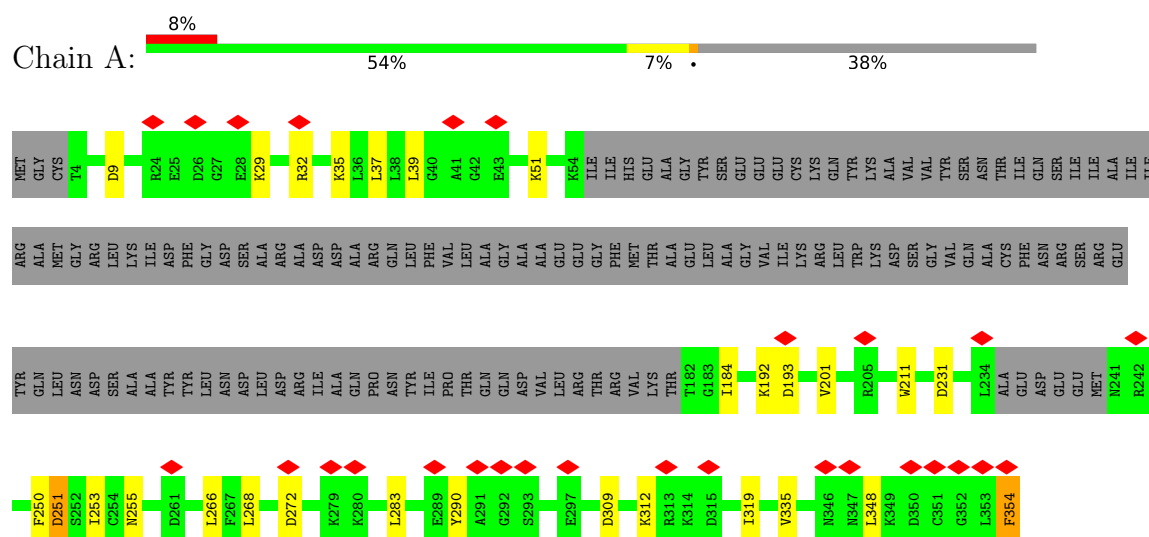
- Molecule 6 is a protein called JMV449.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	6	Total	C	N	O	0	0
			53	38	8	7		

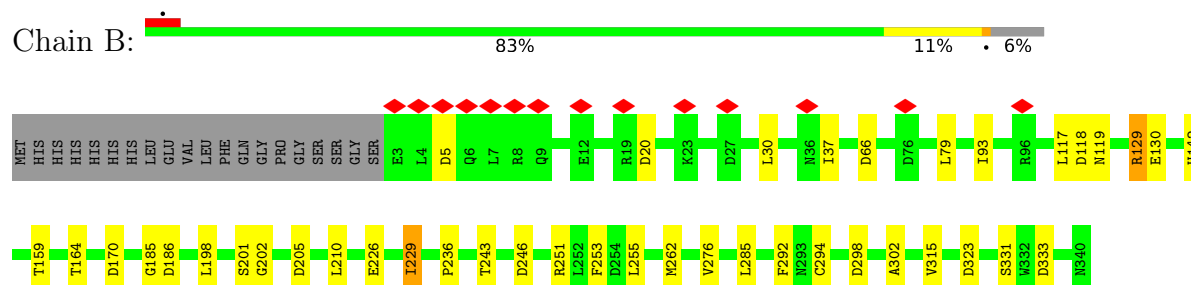
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

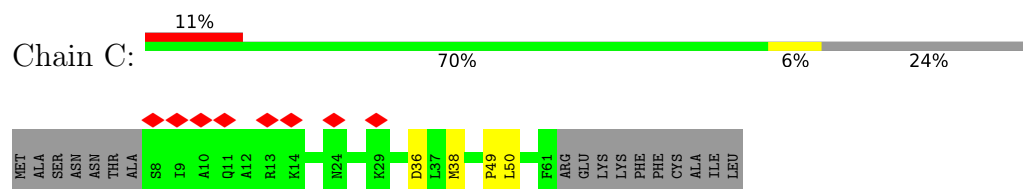
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: scFv16





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146797	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.755	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.308	Depositor
Map size ( $\text{\AA}$ )	163.23334, 163.23334, 163.23334	wwPDB
Map dimensions	118, 118, 118	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3833333, 1.3833333, 1.3833333	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.78	0/1787	1.68	9/2395 (0.4%)
2	B	0.81	0/2632	1.52	19/3570 (0.5%)
3	C	0.76	0/416	1.67	2/562 (0.4%)
4	D	0.81	0/1806	1.37	5/2450 (0.2%)
5	R	1.40	10/2243 (0.4%)	2.26	74/3057 (2.4%)
6	L	0.95	0/54	1.95	0/69
All	All	0.99	10/8938 (0.1%)	1.75	109/12103 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	R	0	6
All	All	0	7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	174	PHE	CG-CD1	39.93	2.22	1.38
5	R	174	PHE	CG-CD2	18.99	1.78	1.38
5	R	332	GLU	CA-CB	-14.12	1.31	1.53
5	R	186	LYS	CB-CG	-9.58	1.23	1.52
5	R	64	VAL	CB-CG1	-8.87	1.23	1.52
5	R	175	LYS	CB-CG	-8.84	1.25	1.52
5	R	71	LEU	CG-CD1	8.26	1.79	1.52
5	R	118	LEU	CG-CD1	-8.04	1.26	1.52
5	R	71	LEU	CG-CD2	7.20	1.76	1.52
5	R	64	VAL	CB-CG2	5.05	1.69	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	174	PHE	CD1-CG-CD2	-30.93	72.20	118.60
5	R	174	PHE	CB-CG-CD1	-18.93	88.52	120.70
5	R	186	LYS	CA-CB-CG	11.97	138.04	114.10
1	A	354	PHE	CA-CB-CG	10.61	124.41	113.80
5	R	118	LEU	CD1-CG-CD2	10.46	133.81	110.80
5	R	71	LEU	CD1-CG-CD2	-9.55	89.80	110.80
5	R	326	PHE	N-CA-CB	8.88	123.17	109.94
5	R	295	VAL	N-CA-CB	8.69	122.35	110.54
5	R	174	PHE	CG-CD2-CE2	8.49	135.13	120.70
5	R	375	PHE	CA-CB-CG	8.35	122.15	113.80
5	R	372	ARG	N-CA-CB	8.23	122.21	109.94
5	R	375	PHE	N-CA-CB	8.22	122.33	110.16
5	R	323	ARG	NE-CZ-NH1	-8.17	113.33	121.50
5	R	366	LEU	N-CA-CB	8.15	121.82	109.91
5	R	188	PHE	CA-CB-CG	8.13	121.93	113.80
4	D	113	GLN	N-CA-CB	7.88	121.71	110.12
5	R	184	ARG	N-CA-CB	7.73	123.32	110.33
5	R	332	GLU	CB-CA-C	7.64	123.47	110.79
5	R	341	PHE	CA-CB-CG	7.61	121.41	113.80
5	R	361	PRO	N-CA-C	7.59	128.10	112.47
5	R	299	ARG	NE-CZ-NH1	-7.58	113.92	121.50
5	R	353	PHE	CA-CB-CG	7.55	121.35	113.80
1	A	335	VAL	N-CA-CB	7.48	118.81	110.51
5	R	371	PHE	N-CA-CB	7.46	121.85	110.44
2	B	118	ASP	CA-CB-CG	7.36	119.96	112.60
2	B	129	ARG	N-CA-CB	7.27	120.64	110.17
5	R	361	PRO	CA-N-CD	-7.26	101.83	112.00
5	R	226	PRO	N-CA-CB	7.02	109.43	103.25
5	R	174	PHE	CA-CB-CG	7.01	120.81	113.80
3	C	49	PRO	N-CA-C	7.01	123.11	113.65
1	A	354	PHE	CB-CA-C	6.98	123.37	110.10
1	A	309	ASP	CA-CB-CG	6.85	119.45	112.60
5	R	64	VAL	CA-CB-CG2	-6.83	98.78	110.40
5	R	127	PHE	CB-CA-C	6.78	120.42	109.02
5	R	159	VAL	N-CA-CB	6.78	118.48	110.55
2	B	323	ASP	CA-CB-CG	6.76	119.36	112.60
5	R	299	ARG	NE-CZ-NH2	6.75	125.27	119.20
2	B	119	ASN	CA-CB-CG	6.60	119.20	112.60
1	A	231	ASP	CA-CB-CG	6.55	119.15	112.60
5	R	313	VAL	N-CA-CB	6.23	117.16	110.62
2	B	205	ASP	CA-CB-CG	6.15	118.75	112.60
2	B	20	ASP	CA-CB-CG	6.13	118.73	112.60
5	R	365	ASN	CB-CA-C	6.13	120.50	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	125	TYR	N-CA-CB	6.04	118.72	109.91
5	R	360	ASN	N-CA-CB	6.03	117.53	110.42
5	R	267	VAL	N-CA-CB	5.99	117.56	110.55
2	B	226	GLU	CB-CG-CD	5.96	122.73	112.60
2	B	246	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	5	ASP	CA-CB-CG	5.94	118.54	112.60
5	R	172	HIS	CB-CA-C	5.94	120.00	111.27
5	R	308	VAL	N-CA-CB	5.88	119.40	110.58
5	R	247	PHE	N-CA-CB	5.88	115.97	110.39
5	R	200	ALA	CA-C-N	5.83	125.00	120.33
5	R	200	ALA	C-N-CA	5.83	125.00	120.33
5	R	239	VAL	CA-CB-CG2	-5.82	100.50	110.40
5	R	325	MET	CG-SD-CE	5.81	113.68	100.90
5	R	359	ILE	CA-C-O	-5.78	115.05	121.17
5	R	187	LYS	CA-CB-CG	5.75	125.59	114.10
1	A	290	TYR	N-CA-CB	-5.70	103.33	110.90
5	R	349	THR	CA-CB-CG2	5.70	120.18	110.50
5	R	180	MET	CA-CB-CG	5.69	125.48	114.10
5	R	90	ARG	NE-CZ-NH1	-5.63	115.86	121.50
1	A	251	ASP	CA-CB-CG	5.63	118.23	112.60
5	R	359	ILE	N-CA-CB	5.58	117.08	110.55
1	A	193	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	253	PHE	CA-CB-CG	5.50	119.30	113.80
5	R	122	VAL	N-CA-CB	5.50	116.39	110.62
5	R	314	VAL	N-CA-CB	5.46	116.94	110.55
1	A	272	ASP	CA-CB-CG	5.46	118.06	112.60
5	R	323	ARG	CD-NE-CZ	5.44	132.02	124.40
5	R	339	TYR	CB-CA-C	5.43	119.80	110.79
5	R	342	TYR	N-CA-CB	5.42	117.87	110.01
5	R	90	ARG	NE-CZ-NH2	5.42	124.07	119.20
5	R	128	ILE	CA-C-N	5.41	131.43	121.70
5	R	128	ILE	C-N-CA	5.41	131.43	121.70
4	D	206	ARG	CA-CB-CG	5.40	124.90	114.10
2	B	201	SER	CA-C-N	5.40	125.32	121.65
2	B	201	SER	C-N-CA	5.40	125.32	121.65
2	B	186	ASP	CA-CB-CG	5.39	117.99	112.60
4	D	73	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	130	GLU	N-CA-CB	5.36	119.55	110.49
5	R	247	PHE	CA-C-N	5.36	124.81	119.24
5	R	247	PHE	C-N-CA	5.36	124.81	119.24
2	B	236	PRO	N-CA-C	5.35	120.79	113.84
5	R	98	GLN	N-CA-CB	5.33	117.88	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	68	PHE	CA-CB-CG	5.32	119.12	113.80
3	C	36	ASP	CA-CB-CG	5.32	117.92	112.60
4	D	103	TYR	N-CA-CB	5.24	118.19	109.60
5	R	365	ASN	CA-CB-CG	5.24	117.84	112.60
5	R	172	HIS	CA-CB-CG	5.21	119.01	113.80
2	B	66	ASP	CA-CB-CG	5.20	117.80	112.60
5	R	332	GLU	CA-CB-CG	5.20	124.50	114.10
2	B	292	PHE	CA-CB-CG	5.20	119.00	113.80
5	R	114	LEU	CA-C-O	-5.18	115.38	120.82
5	R	313	VAL	O-C-N	5.17	127.54	121.96
5	R	142	ARG	N-CA-CB	5.15	117.48	110.01
2	B	170	ASP	CA-CB-CG	5.15	117.75	112.60
5	R	332	GLU	N-CA-CB	-5.13	102.58	110.12
5	R	75	VAL	N-CA-CB	5.12	116.54	110.55
5	R	172	HIS	CA-C-O	-5.11	115.66	121.28
5	R	120	MET	CG-SD-CE	5.11	112.13	100.90
5	R	360	ASN	CA-CB-CG	5.08	117.68	112.60
5	R	115	THR	N-CA-CB	5.05	117.50	109.82
5	R	246	ILE	CA-C-O	-5.05	115.31	120.71
2	B	298	ASP	CA-CB-CG	5.05	117.65	112.60
5	R	129	TRP	N-CA-CB	5.05	119.08	110.50
5	R	367	VAL	CA-CB-CG1	5.04	118.98	110.40
5	R	164	VAL	N-CA-CB	5.04	116.45	110.55
5	R	240	ASN	O-C-N	5.01	127.24	122.03

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	251	ARG	Sidechain
5	R	127	PHE	Peptide
5	R	174	PHE	Sidechain
5	R	182	ARG	Sidechain
5	R	299	ARG	Sidechain
5	R	323	ARG	Sidechain
5	R	90	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1758	0	1755	8	0
2	B	2585	0	2479	14	0
3	C	410	0	421	2	0
4	D	1762	0	1696	10	0
5	R	2190	0	2258	67	0
6	L	53	0	63	1	0
All	All	8758	0	8672	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:174:PHE:CD2	5:R:174:PHE:CG	1.78	1.66
5:R:71:LEU:CD2	5:R:71:LEU:CG	1.76	1.61
5:R:71:LEU:CG	5:R:71:LEU:CD1	1.79	1.56
5:R:174:PHE:CG	5:R:174:PHE:CD1	2.22	1.27
5:R:174:PHE:CD2	5:R:174:PHE:CD1	2.39	1.04
5:R:71:LEU:CD2	5:R:71:LEU:CD1	2.51	0.89
5:R:304:VAL:HG22	5:R:363:LEU:HD21	1.57	0.87
5:R:142:ARG:NH1	5:R:226:PRO:HA	1.93	0.84
5:R:142:ARG:HH12	5:R:226:PRO:HA	1.47	0.79
5:R:174:PHE:CD1	5:R:174:PHE:CB	2.66	0.79
5:R:71:LEU:CD1	5:R:71:LEU:CB	2.63	0.75
5:R:237:ILE:HD12	5:R:326:PHE:CE2	2.24	0.72
2:B:37:ILE:HD11	3:C:38:MET:HE3	1.73	0.71
5:R:237:ILE:HD12	5:R:326:PHE:HE2	1.56	0.70
5:R:362:ILE:HG22	5:R:366:LEU:HD23	1.73	0.70
5:R:237:ILE:CD1	5:R:326:PHE:CE2	2.78	0.66
2:B:229:ILE:HD12	2:B:243:THR:HG23	1.76	0.65
5:R:237:ILE:CD1	5:R:326:PHE:HE2	2.10	0.65
5:R:174:PHE:CD1	5:R:174:PHE:HB3	2.34	0.61
5:R:67:THR:HG23	5:R:124:LEU:HD11	1.82	0.60
5:R:164:VAL:HA	5:R:255:LEU:HD13	1.85	0.58
5:R:180:MET:HG3	5:R:184:ARG:HH11	1.70	0.57
1:A:250:PHE:CE1	1:A:266:LEU:HD11	2.41	0.56
5:R:186:LYS:NZ	5:R:189:ILE:HD12	2.20	0.56
5:R:315:CYS:HG	5:R:316:TRP:CD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD13	1:A:319:ILE:HG23	1.88	0.55
5:R:71:LEU:HA	5:R:71:LEU:HD13	1.89	0.54
5:R:345:PHE:O	5:R:349:THR:HG23	2.09	0.53
5:R:118:LEU:HD12	5:R:151:CYS:SG	2.49	0.53
5:R:125:TYR:CE1	5:R:126:ASN:HB3	2.44	0.53
4:D:175:LEU:HD21	4:D:178:TYR:HB3	1.90	0.53
1:A:211:TRP:HB2	2:B:117:LEU:HD21	1.91	0.53
4:D:83:MET:HE1	4:D:117:LEU:HD13	1.91	0.52
5:R:304:VAL:CG1	5:R:363:LEU:HD11	2.39	0.52
5:R:304:VAL:HG13	5:R:363:LEU:HD11	1.91	0.52
5:R:74:PHE:HB2	5:R:120:MET:HE2	1.92	0.51
5:R:326:PHE:CE1	6:L:12:ILE:HD13	2.46	0.51
5:R:71:LEU:CD2	5:R:71:LEU:CB	2.80	0.50
5:R:168:LEU:HD22	5:R:172:HIS:CE1	2.47	0.50
4:D:91:THR:HG23	4:D:118:THR:HA	1.93	0.50
2:B:37:ILE:HD11	3:C:38:MET:CE	2.42	0.50
2:B:331:SER:OG	2:B:333:ASP:OD1	2.30	0.49
4:D:5:VAL:HG13	4:D:113:GLN:HE22	1.77	0.49
5:R:174:PHE:O	5:R:177:LYS:HB2	2.12	0.49
1:A:184:ILE:CD1	1:A:201:VAL:HG23	2.43	0.48
4:D:39:GLN:HB2	4:D:45:LEU:HD23	1.95	0.48
5:R:115:THR:HG22	5:R:151:CYS:HB3	1.96	0.47
5:R:340:ASP:HA	5:R:343:HIS:ND1	2.29	0.47
5:R:126:ASN:HA	5:R:129:TRP:HA	1.96	0.47
5:R:371:PHE:HA	5:R:374:ILE:HB	1.96	0.47
1:A:348:LEU:HD11	5:R:298:LEU:HD23	1.96	0.46
2:B:276:VAL:HG13	2:B:285:LEU:HD21	1.96	0.46
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.49	0.46
5:R:226:PRO:CG	5:R:233:VAL:HG21	2.46	0.46
5:R:329:ILE:HG23	5:R:333:GLN:HB2	1.97	0.46
5:R:160:ALA:HB1	5:R:251:VAL:HG21	1.98	0.46
5:R:156:ALA:HB1	5:R:248:PRO:HG2	1.97	0.46
2:B:202:GLY:HA3	2:B:229:ILE:HD11	1.98	0.45
2:B:210:LEU:HD22	2:B:255:LEU:HD12	1.97	0.45
5:R:71:LEU:CD1	5:R:71:LEU:HA	2.46	0.45
5:R:237:ILE:CD1	5:R:326:PHE:CD2	2.99	0.45
5:R:371:PHE:HA	5:R:374:ILE:H	1.82	0.45
4:D:92:ALA:HB3	4:D:94:TYR:HE1	1.82	0.45
5:R:105:LEU:HD12	5:R:162:LEU:HD21	1.99	0.45
2:B:198:LEU:HD12	2:B:210:LEU:HD11	1.99	0.45
5:R:186:LYS:HZ1	5:R:189:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ARG:HH12	4:D:199:ALA:HB2	1.81	0.44
5:R:142:ARG:HH12	5:R:226:PRO:CA	2.22	0.44
2:B:79:LEU:HD12	2:B:93:ILE:HD12	1.99	0.44
5:R:336:PRO:HA	5:R:339:TYR:CD2	2.53	0.44
2:B:262:MET:HE2	2:B:302:ALA:HB2	1.99	0.43
5:R:304:VAL:HG22	5:R:363:LEU:CD2	2.40	0.43
5:R:86:PHE:HD1	5:R:90:ARG:HH11	1.66	0.43
5:R:172:HIS:HD2	5:R:175:LYS:NZ	2.17	0.43
5:R:226:PRO:HG3	5:R:233:VAL:HG21	2.01	0.42
2:B:164:THR:HG22	2:B:185:GLY:C	2.44	0.42
5:R:180:MET:HG3	5:R:184:ARG:HE	1.83	0.42
2:B:294:CYS:SG	2:B:315:VAL:HG11	2.60	0.42
5:R:320:HIS:ND1	5:R:323:ARG:HD3	2.33	0.42
5:R:363:LEU:HD22	5:R:366:LEU:HD11	2.01	0.42
5:R:123:GLU:HG2	5:R:354:TYR:OH	2.20	0.41
5:R:172:HIS:HD1	5:R:176:ALA:HB2	1.84	0.41
5:R:126:ASN:C	5:R:129:TRP:HA	2.45	0.41
5:R:167:TYR:N	5:R:259:ILE:HD11	2.35	0.41
2:B:30:LEU:HD23	2:B:262:MET:SD	2.61	0.41
1:A:39:LEU:HD13	1:A:253:ILE:HG21	2.02	0.41
1:A:354:PHE:HB3	5:R:367:VAL:HG11	2.03	0.41
5:R:97:LEU:HD21	5:R:177:LYS:HG2	2.01	0.41
4:D:12:VAL:HG11	4:D:86:LEU:HD12	2.03	0.41
5:R:65:LEU:O	5:R:69:VAL:HG23	2.21	0.41
5:R:97:LEU:HD13	5:R:179:LEU:HG	2.03	0.41
4:D:177:ILE:HA	4:D:182:ASN:O	2.22	0.40
5:R:228:ILE:HG23	5:R:232:THR:HB	2.02	0.40
4:D:126:ILE:HD11	4:D:222:GLU:OE2	2.21	0.40
5:R:180:MET:HG3	5:R:184:ARG:NH1	2.37	0.40
5:R:306:ARG:HA	5:R:309:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.



The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/354 (60%)	203 (96%)	9 (4%)	0	100	100
2	B	336/358 (94%)	328 (98%)	8 (2%)	0	100	100
3	C	52/71 (73%)	52 (100%)	0	0	100	100
4	D	227/259 (88%)	219 (96%)	8 (4%)	0	100	100
5	R	268/436 (62%)	254 (95%)	14 (5%)	0	100	100
6	L	4/6 (67%)	1 (25%)	3 (75%)	0	100	100
All	All	1099/1484 (74%)	1057 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/305 (64%)	184 (95%)	10 (5%)	21	54
2	B	278/298 (93%)	274 (99%)	4 (1%)	59	77
3	C	43/58 (74%)	42 (98%)	1 (2%)	44	70
4	D	191/209 (91%)	180 (94%)	11 (6%)	18	51
5	R	238/368 (65%)	190 (80%)	48 (20%)	1	7
6	L	6/6 (100%)	5 (83%)	1 (17%)	2	11
All	All	950/1244 (76%)	875 (92%)	75 (8%)	13	40

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	29	LYS
1	A	32	ARG
1	A	35	LYS

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Mol	Chain	Res	Type
1	A	37	LEU
1	A	51	LYS
1	A	192	LYS
1	A	268	LEU
1	A	283	LEU
1	A	312	LYS
2	B	129	ARG
2	B	142	HIS
2	B	159	THR
2	B	229	ILE
3	C	50	LEU
4	D	11	LEU
4	D	43	LYS
4	D	51	ILE
4	D	113	GLN
4	D	117	LEU
4	D	147	CYS
4	D	148	ARG
4	D	151	LYS
4	D	154	LEU
4	D	179	ARG
4	D	232	LYS
5	R	92	LYS
5	R	94	LEU
5	R	97	LEU
5	R	98	GLN
5	R	99	SER
5	R	110	LEU
5	R	123	GLU
5	R	125	TYR
5	R	129	TRP
5	R	142	ARG
5	R	152	THR
5	R	155	THR
5	R	162	LEU
5	R	170	ILE
5	R	172	HIS
5	R	175	LYS
5	R	178	THR
5	R	179	LEU
5	R	184	ARG
5	R	186	LYS

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Mol	Chain	Res	Type
5	R	187	LYS
5	R	188	PHE
5	R	192	ILE
5	R	198	LEU
5	R	225	THR
5	R	261	ASN
5	R	305	LEU
5	R	324	LEU
5	R	329	ILE
5	R	330	SER
5	R	332	GLU
5	R	334	TRP
5	R	335	THR
5	R	337	PHE
5	R	338	LEU
5	R	339	TYR
5	R	341	PHE
5	R	342	TYR
5	R	357	SER
5	R	359	ILE
5	R	361	PRO
5	R	365	ASN
5	R	366	LEU
5	R	368	SER
5	R	370	ASN
5	R	373	HIS
5	R	375	PHE
5	R	376	LEU
6	L	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	333	GLN
2	B	176	GLN
2	B	220	GLN
2	B	225	HIS
2	B	259	GLN
3	C	18	GLN
4	D	39	GLN
4	D	113	GLN

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Mol	Chain	Res	Type
4	D	167	GLN
5	R	102	HIS
5	R	126	ASN
5	R	172	HIS
5	R	296	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

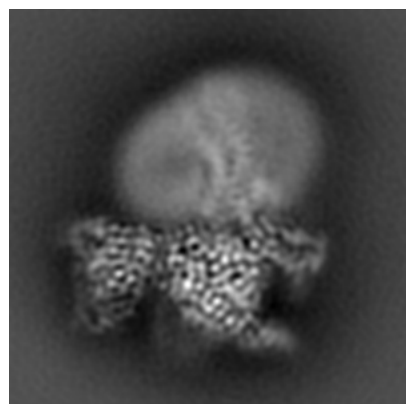
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64911. These allow visual inspection of the internal detail of the map and identification of artifacts.

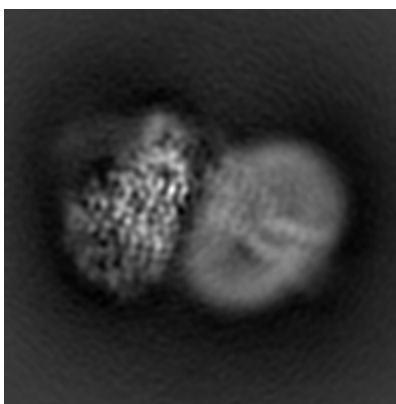
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

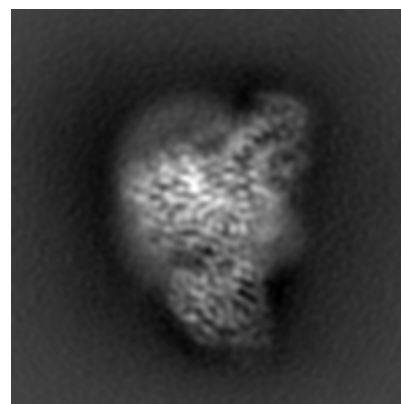
#### 6.1.1 Primary map



X

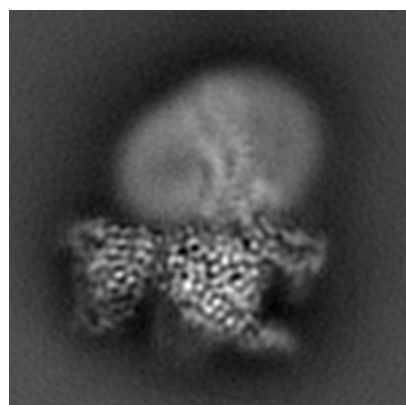


Y

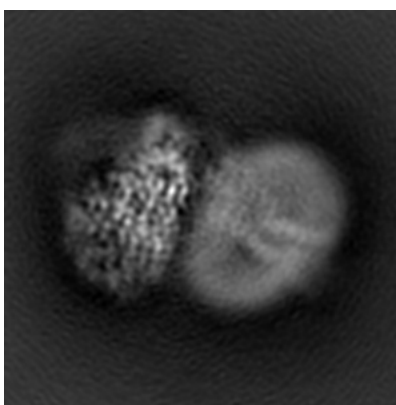


Z

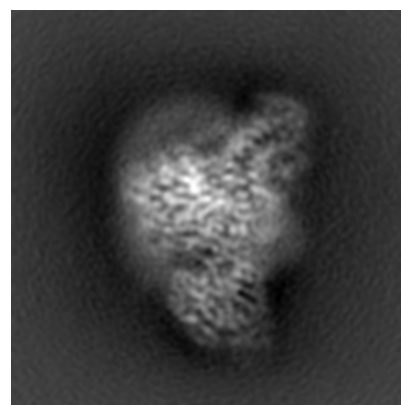
#### 6.1.2 Raw map



X



Y

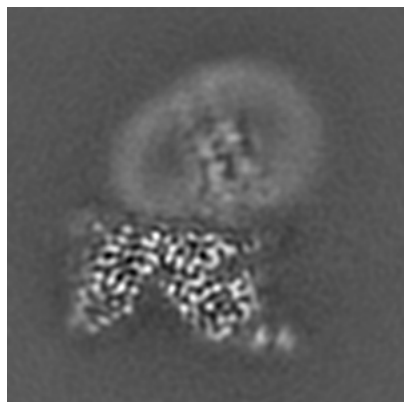


Z

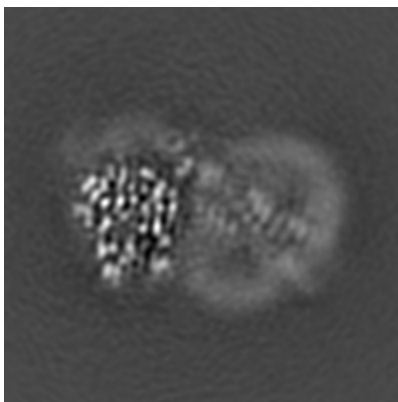
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

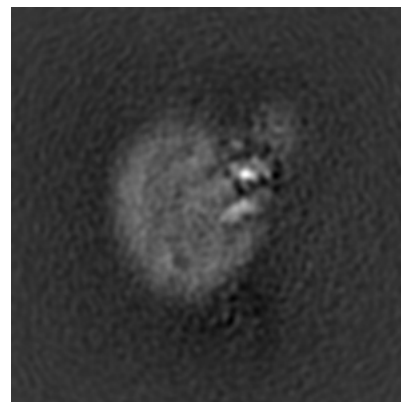
### 6.2.1 Primary map



X Index: 59

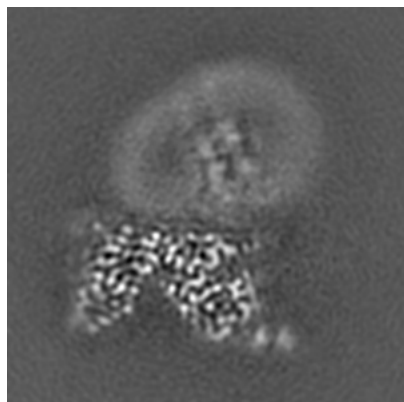


Y Index: 59

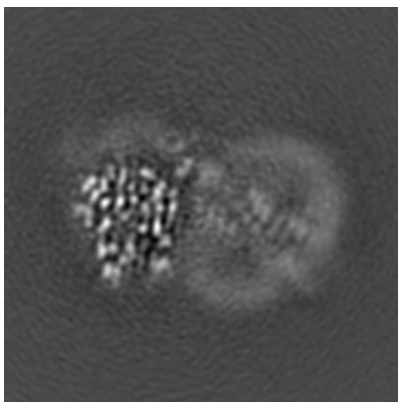


Z Index: 59

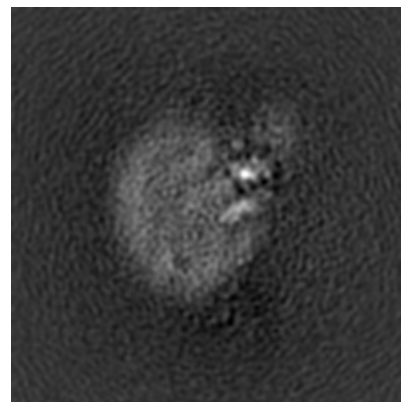
### 6.2.2 Raw map



X Index: 59



Y Index: 59

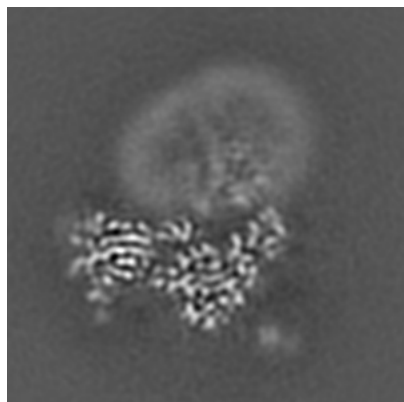


Z Index: 59

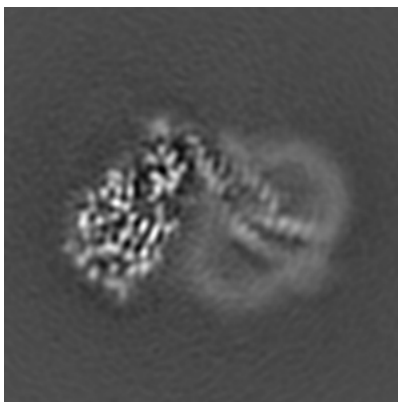
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

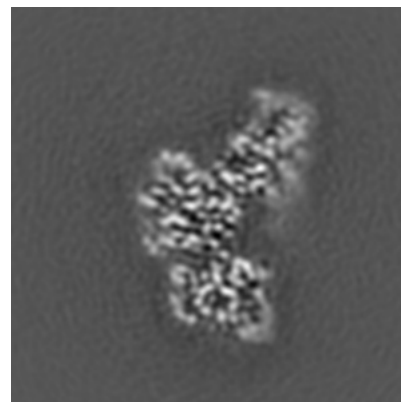
### 6.3.1 Primary map



X Index: 65

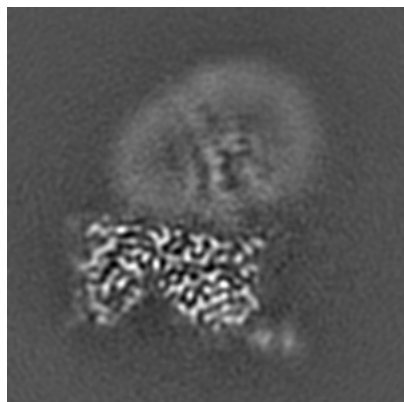


Y Index: 67

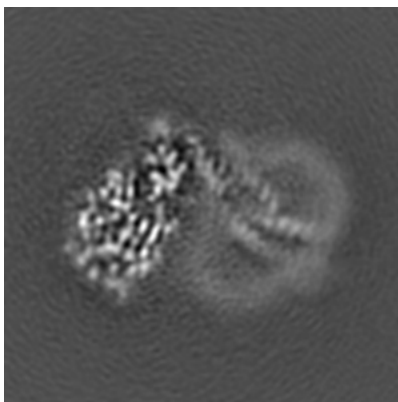


Z Index: 45

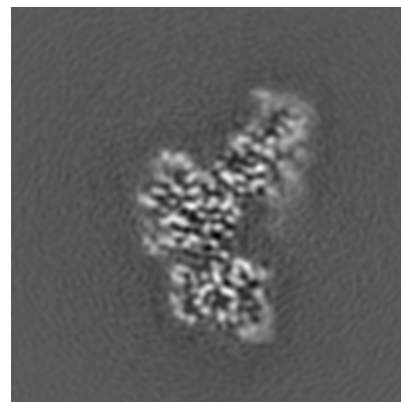
### 6.3.2 Raw map



X Index: 61



Y Index: 67

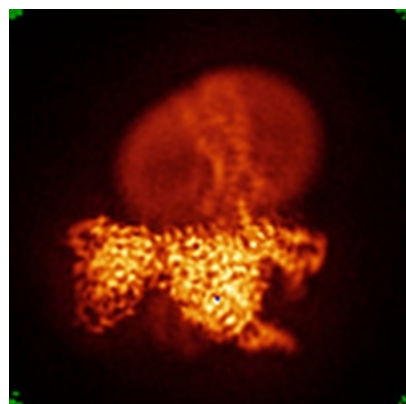


Z Index: 45

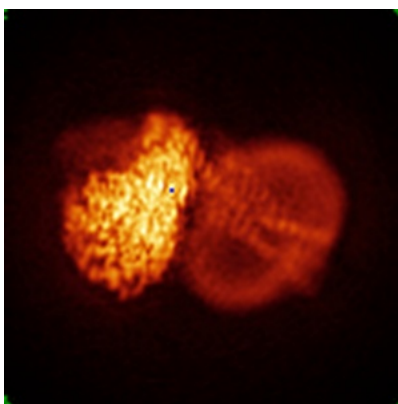
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

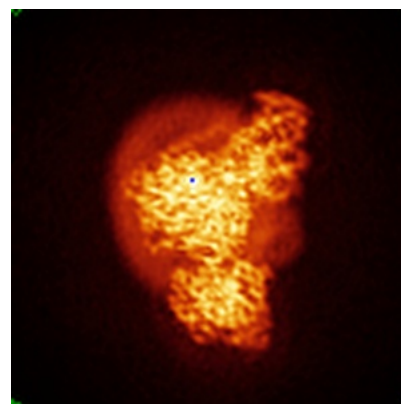
### 6.4.1 Primary map



X

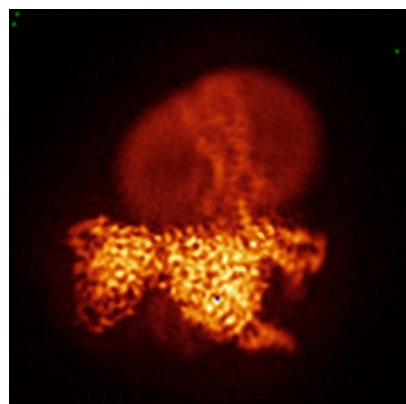


Y

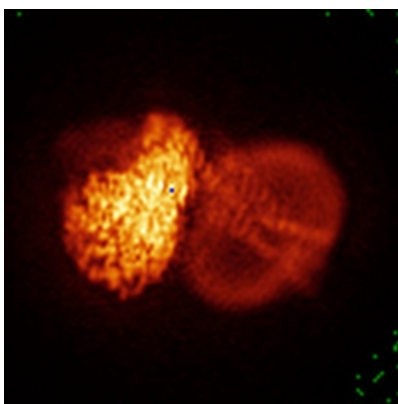


Z

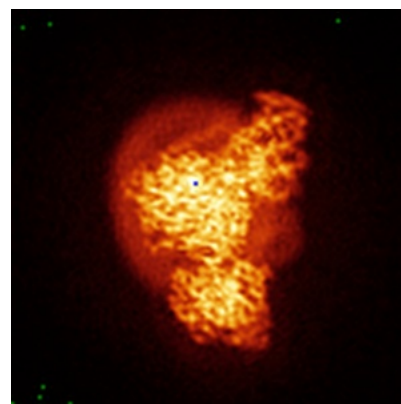
### 6.4.2 Raw map



X



Y



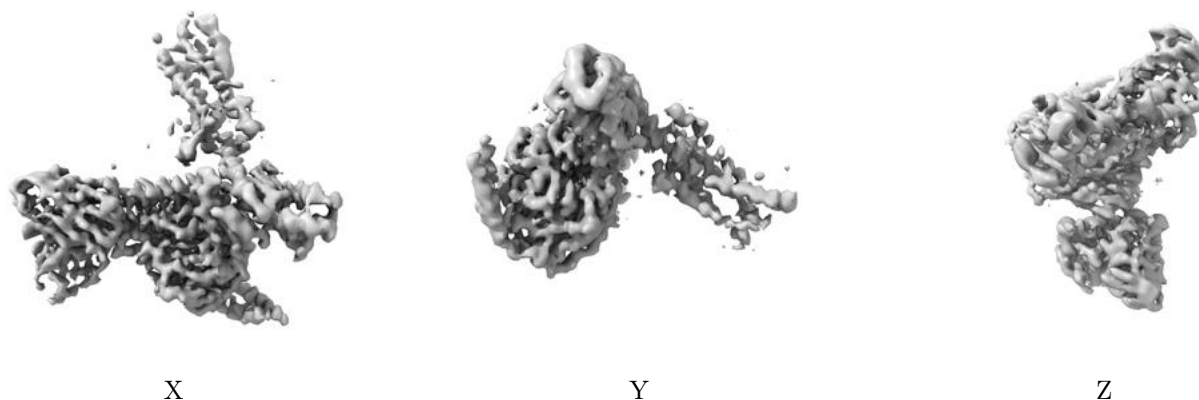
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



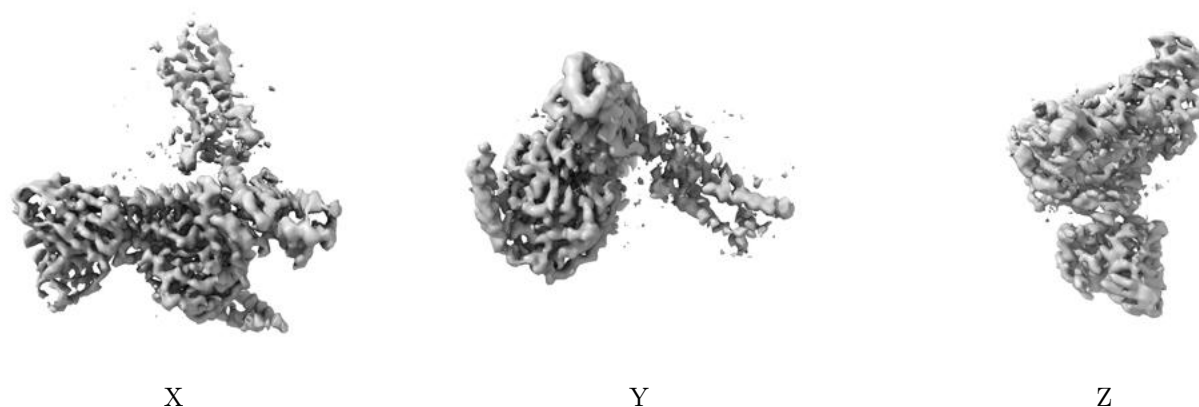
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.308. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

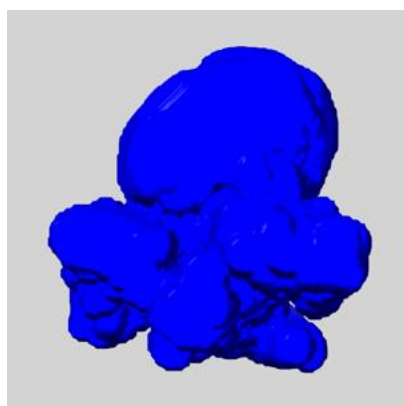
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

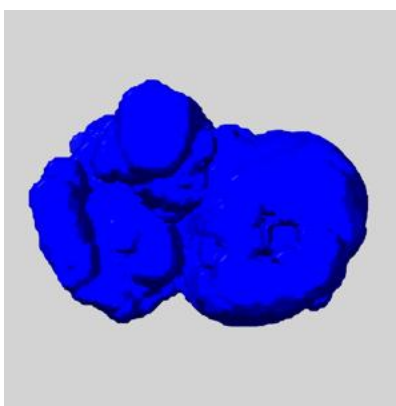
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

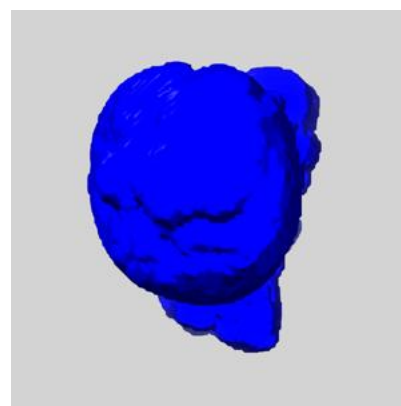
### 6.6.1 emd\_64911\_msk\_1.map [i](#)



X



Y

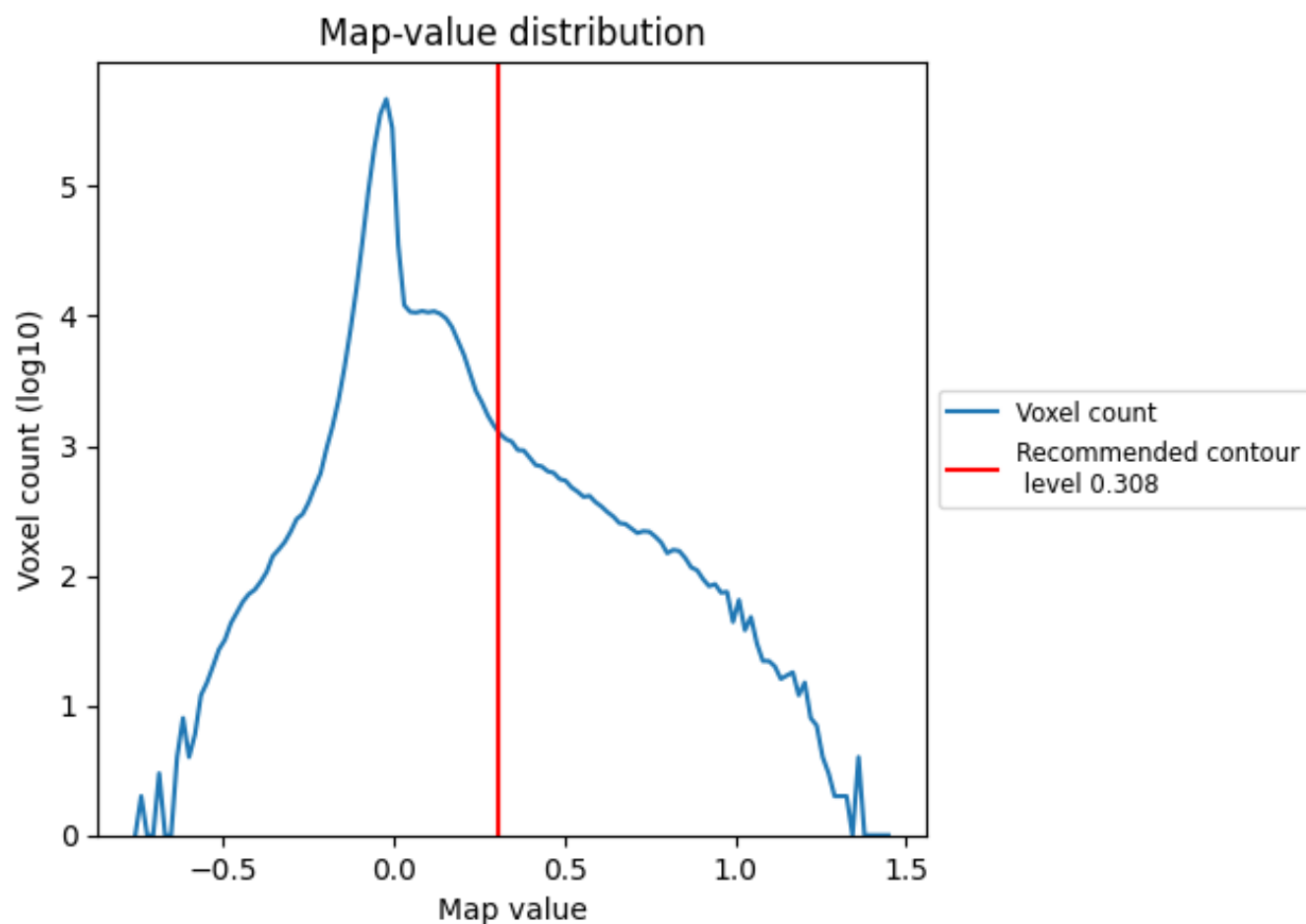


Z

## 7 Map analysis [i](#)

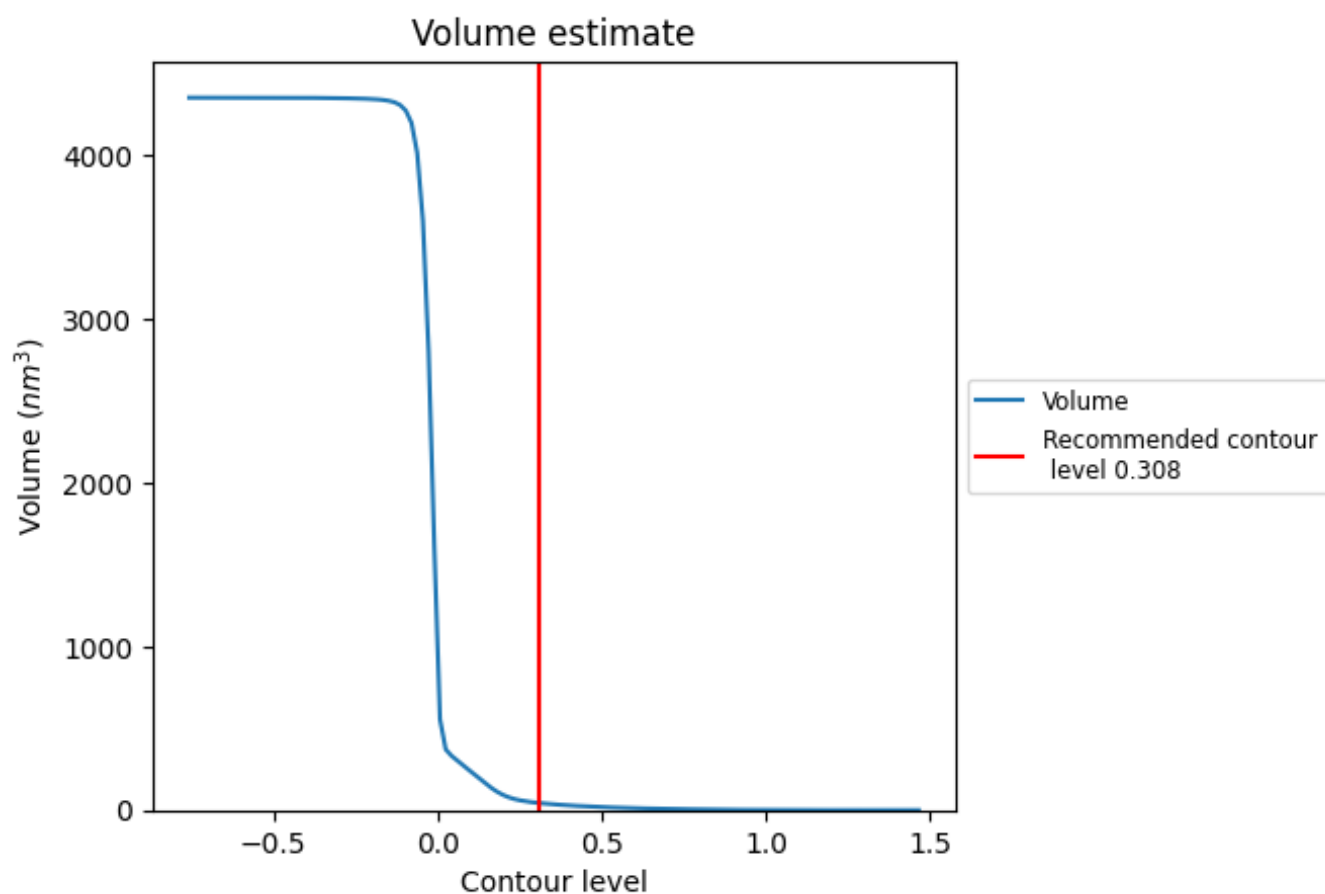
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

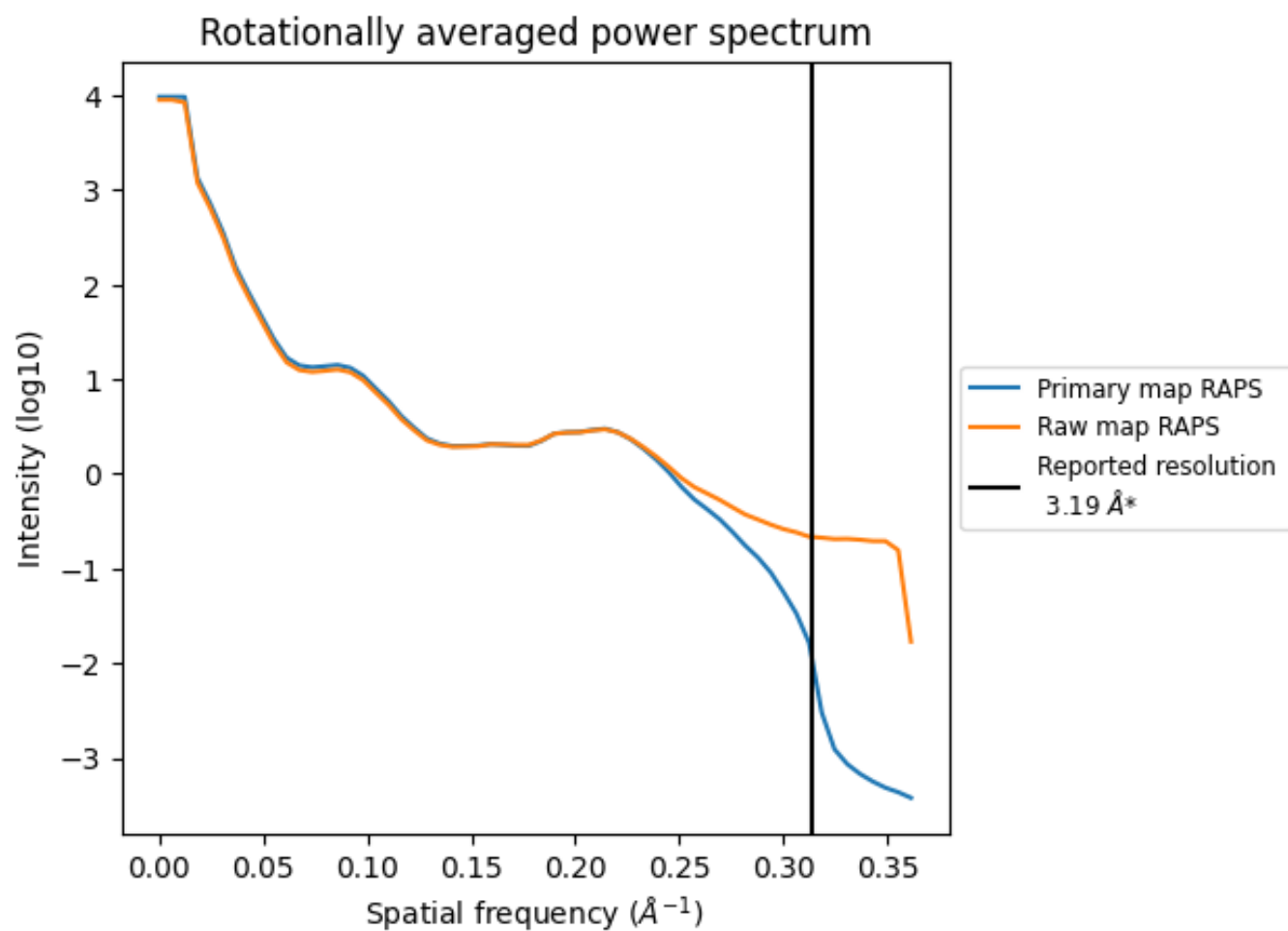
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm<sup>3</sup>; this corresponds to an approximate mass of 40 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

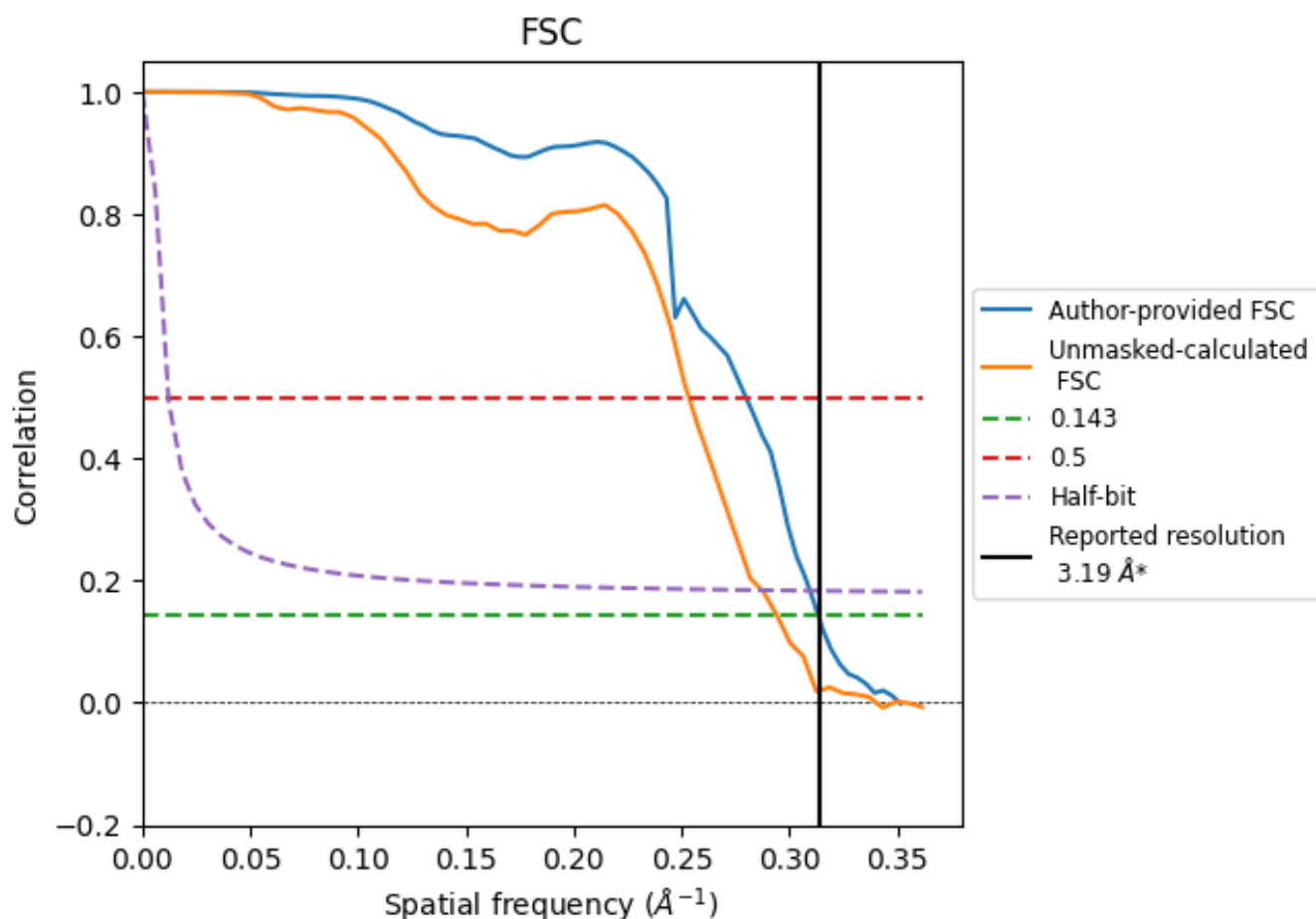


\*Reported resolution corresponds to spatial frequency of 0.313  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.313  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

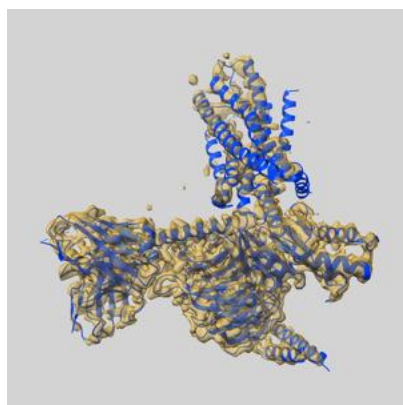
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.19	3.58	3.23
Unmasked-calculated*	3.40	3.95	3.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

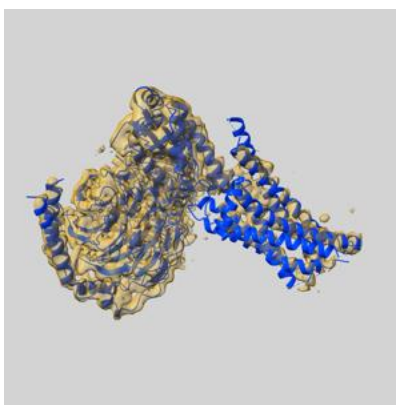
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64911 and PDB model 9VB0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

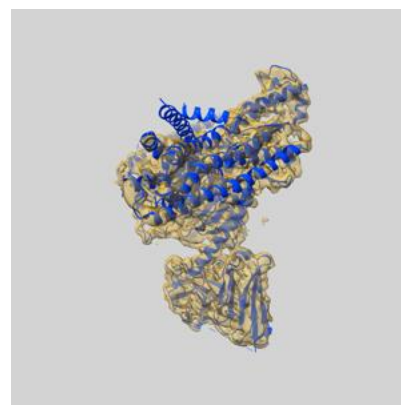
### 9.1 Map-model overlay [i](#)



X



Y

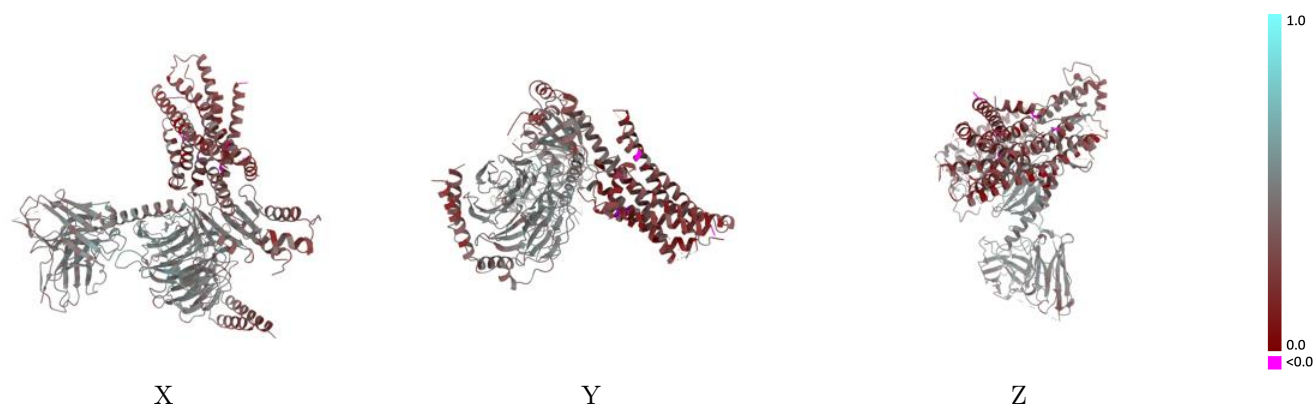


Z

The images above show the 3D surface view of the map at the recommended contour level 0.308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

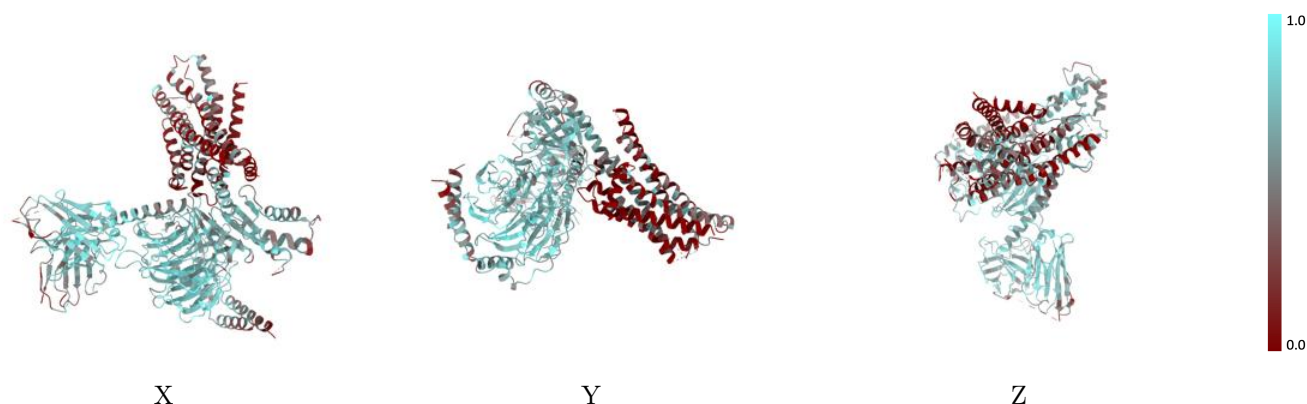


## 9.2 Q-score mapped to coordinate model [i](#)



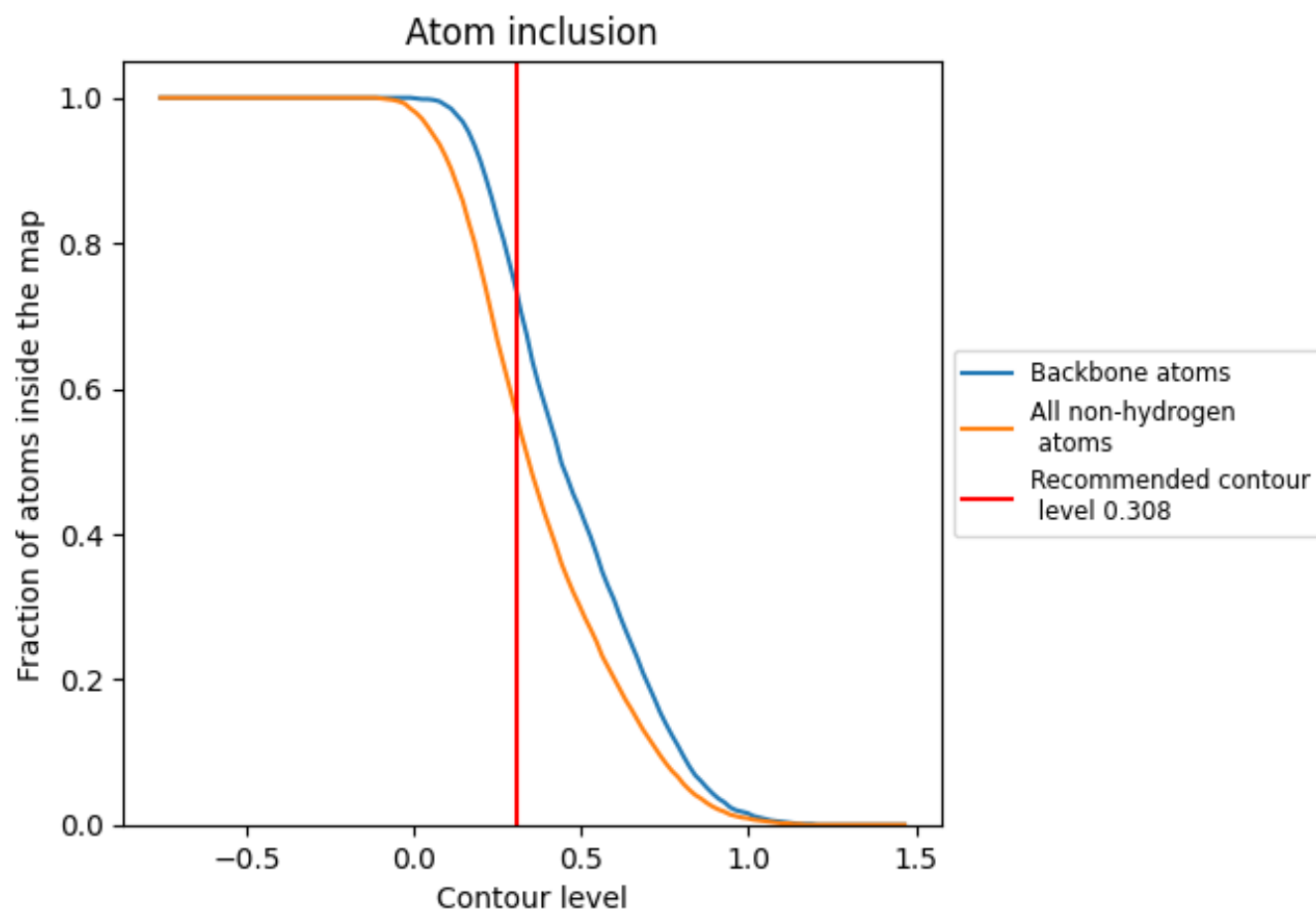
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.308).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5630	<div></div> 0.3880
A	<div></div> 0.5960	<div></div> 0.4000
B	<div></div> 0.7500	<div></div> 0.4600
C	<div></div> 0.6030	<div></div> 0.3890
D	<div></div> 0.6780	<div></div> 0.4640
L	<div></div> 0.2690	<div></div> 0.2880
R	<div></div> 0.2210	<div></div> 0.2340

1.0

0.0

<0.0